Target Gas Density Calculator Concept, Usage & Limitations

NIF Users' Forum

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Originally authored by Jim Fair, PhD Mac conversion by Curtis Walters, PhD





Why Have a Gas Density Calculator?

- In 2012, it was realized that the non-ideality of subcritical THD gas mixtures exceeded the allowable uncertainty of the capsule density.
 - Why? Conversion from density to pressure was not accurate using the Ideal Gas Law alone.
 - Jim Fair authored the first calculator that calculated the density of the isotopic mixtures of hydrogen and helium.
 - Other gases & gas mixtures being shot are similarly non-ideal. E.g., Neopentane.

Primary purpose

- To calculate an accurate conversion of density (mg/cm³) to pressure (torr) in target gas fill requests.
 - To quantify the non-ideal behavior of subcritical or high pressure gases and gas mixtures.
- Secondary purposes
 - To predict the equilibrium of THD mixtures (H₂, D₂, T₂, HD, HT, DT) from cryogenic to room temperature.
 - To predict the atomic particle density (atoms/cm³).



Model Approach To Non-Ideality Corrections

Virial Coefficient Corrections to the Ideal Gas Law

$$-z = \frac{P}{RT\rho_m} \approx 1 + B\rho_m + C\rho_m^2 + \dots$$

- Mixing Rules (generally accepted for B, but not universally accepted for C)
 - 2nd Virial Coefficient for low pressure, low temp or moderate pressure, high temperature gases

$$-B_{ij} = \frac{(B_i + B_j)}{2}$$

$$-B_{mix} = \sum_{i=1}^{N} y_i B_{ii} + \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} y_i y_j \delta_{ij}$$

$$-\delta_{ij} = 2B_{ij} - B_{ii} - B_{jj}$$

• 3rd Virial Coefficient – for high pressure gases near critical temperature

$$-C_{ijk} = \frac{(c_i + c_j + c_k)}{3} -C_{mix} = \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{k=1}^{N} y_i y_j y_k C_{ijk}$$

Caveats

- How good are the predictions? As good as the data.
 - E.g., Vapor pressure. Sources include:
 - Correlations from NIST
 - Compilation of literature data polynomial fit
 - Antoine equation
 - THD Virial Coefficients
 - 2nd VC High Confidence:
 - From PIMC models, which match historical data from Souers, Sherwood, Reed, Grilly and others, and is valid from 15K through RT.
 - 3rd VC Unproven:
 - Is estimated using H_2 3rd VC data and a corresponding states mapping (about T_r) from the 2nd VCs.
- Programming sanity checks is time consuming
 - Use your own judgment and knowledge of the materials being studied.
 - When in doubt, call me.

Using the Density Calculator (Demo)

V2.5 & above:

- On a PC: Open the document, accept that Macros need to be run.
- Navigate to the "Calculator" tab.
- Enter the desired mass density & shot temperature.
- Adjust the composition.
- Check the right hand fields.
- Find the pressure alongside the desired composition

V2.4 (Mac)

- Open the document.
- Navigate to the "Calculator" tab.
- Enter the desired mass density & shot temperature
- Adjust the composition.
- For THD Mixtures ONLY:
 - N.B. Click the "THD Mixture Calculate" button. Wait for convergence.
 - If there is no convergence, navigate to the "THD EquilibriumCalculator" tab
 Click "Reset" and "Solve" buttons.

 - Adjust "initial value factor" if necessary.
 - Re-click "Solve" to increase the number of solver iterations.
- Check the right hand fields.
- Find the pressure alongside the desired composition
- V2.6 beta
 - Working to resolve the issue of porting VB from PC to Mac version.



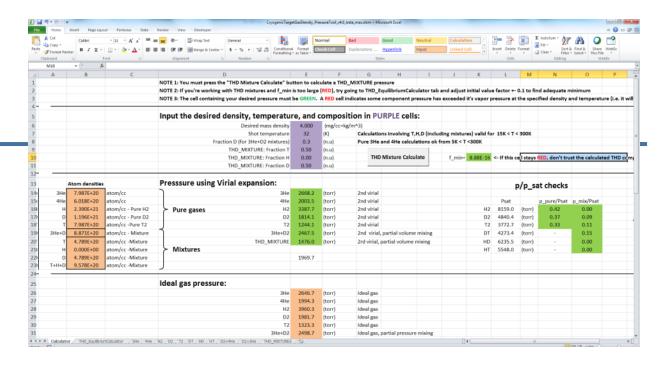


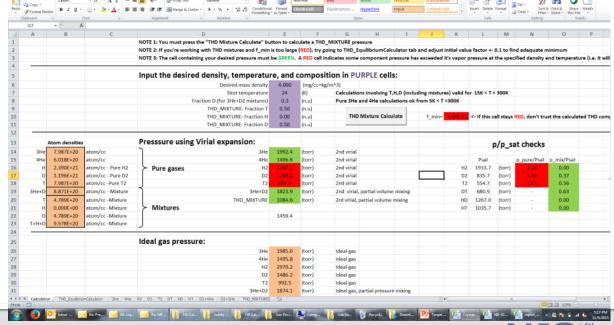
Using the Density Calculator (Demo)

- Case 1: Recent D₂-Filled HDC Symcap shot (N151025-001)
- Case 2: How do I request a specific density/mixture?
- Case 3: Post shot re-verification

Using the Density Calculator – Case 1

- Recent D₂-Filled HDC Symcap shot (N151025-001)
 - Original desired density:
 - 4 mg/cc at 32K
 - AppMan Request
 - 1486 Torr at 24K
 - Fielded Capsule
 - Liquid Deuterium
 - What red flags existed?









Using the Density Calculator (Case 2)

- Case 2: How do I request a specific density/mixture?
 - 10 mg/cc of D₂ at 32K
 - Answer should be immediately available
 - $10 \text{ mg/cc of } 0.4 \text{ at}\% \text{ D-}^{3}\text{He at } 32\text{K}$
 - 10 mg/cc of 50:50 DT at 32K
 - Mac: must click solver button
 - 10 mg/cc of 2/24/74 HDT at 32K
 - Mac: must click solver button

Using the Density Calculator (Demo)

- Case 3: Post shot analysis
 - Requested: 10 mg/cc of 0.75/0.25 HT at 32K
 - Calculator indicates: 5022 Torr at 32K.
 - Cryo Reports on !DATA:
 - 5069 Torr
 - Mass Spec Analysis
 - 74% H
 - 25% T
 - 1% D
 - Calculator (trial & error)
 - 10.21 mg/cc at 32K
 - NOTE: 75/25 from calculator is 10.13 mg/cc

Current ELM Version is NIF-0135638-AF or v2.5

- Recently added/changed features
 - On the PC version, the THD Equilibrium Calculator is now "live," no need to hit a reset & run-macro button
 - Seems to work for three-component THD mixtures.
 - Uses a pragmatic "forced-mass-balance" scheme to converge the equilibrium expressions.
 - Science fiction checks
 - Polynomial correlation of saturated vapor density of THD.
 - Color coding: an indication of when an estimate is violating something
 - Green is good
 - Red is bad
 - Any other color: Use with Caution
 - Data may be extrapolated or near some critical value (e.g., saturation temp, valid range of vapor pressure expression, etc.)
- If its broken, or if the calculator doesn't have a mixture or material that is of interest, contact me.